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Components: 1. Methyl ethanoate, $C_2H_6O_2$ /70-20-9/
2. 1-Butanol, $C_4H_{10}O$ /71-36-3/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

x_i , mole fraction of component i in liquid phase

y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain)

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SOURCE OF DATA

Susial, P.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 74.66$						$P/kPa = 127.99$											
x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1
0.0000	381.87	0.0000	0.4524	334.82	0.9206	0.0000	397.02	0.0000	0.4996	350.63	0.9041						
0.0035	381.16	0.0340	0.4845	333.71	0.9275	0.0211	393.45	0.1388	0.5333	349.54	0.9134						
0.0068	380.39	0.0640	0.5179	332.72	0.9334	0.0431	389.73	0.2585	0.5518	348.82	0.9185						
0.0128	379.05	0.1150	0.5455	331.81	0.9389	0.0548	387.90	0.3123	0.5878	347.42	0.9200						
0.0215	377.14	0.1829	0.5798	330.86	0.9448	0.0668	385.97	0.3627	0.5957	347.02	0.9290						
0.0321	374.93	0.2562	0.6146	329.95	0.9500	0.0828	383.68	0.4243	0.6318	346.30	0.9363						
0.0421	372.97	0.3183	0.6455	329.15	0.9542	0.0991	381.41	0.4774	0.6610	345.37	0.9422						
0.0608	369.46	0.4189	0.6814	328.27	0.9590	0.1168	379.06	0.5287	0.6931	344.48	0.9479						
0.0696	367.93	0.4588	0.7189	327.44	0.9638	0.1509	374.79	0.6108	0.7215	343.65	0.9533						
0.0813	365.92	0.5067	0.7459	326.73	0.9673	0.2107	369.17	0.7104	0.7552	342.77	0.9595						
0.0944	363.79	0.5546	0.7784	326.12	0.9709	0.2356	366.80	0.7430	0.7888	341.95	0.9649						
0.1210	359.82	0.6353	0.8086	325.44	0.9745	0.2617	364.51	0.7725	0.8178	341.13	0.9699						
0.1837	351.84	0.7623	0.8440	324.65	0.9788	0.2880	362.45	0.7949	0.8548	340.20	0.9757						
0.2036	349.91	0.7878	0.8749	323.98	0.9825	0.3088	360.78	0.8126	0.8821	339.54	0.9797						
0.2255	347.84	0.8106	0.9039	323.39	0.9860	0.3381	358.81	0.8330	0.9117	338.87	0.9845						
0.2484	346.02	0.8301	0.9282	322.88	0.9892	0.3627	357.40	0.8478	0.9355	338.26	0.9884						
0.2657	344.63	0.8435	0.9504	322.38	0.9924	0.3898	355.85	0.8620	0.9581	337.69	0.9922						
0.2924	342.70	0.8605	0.9670	321.99	0.9945	0.4153	354.56	0.8728	0.9776	337.18	0.9955						
0.3242	340.82	0.8770	0.9795	321.70	0.9965	0.4299	353.68	0.8796	0.9916	336.83	0.9980						
0.3570	338.96	0.8918	0.9909	321.44	0.9981	0.4600	352.43	0.8903	1.0000	336.60	1.0000						
0.3889	337.47	0.9026	1.0000	321.21	1.0000												
0.4186	336.19	0.9119															

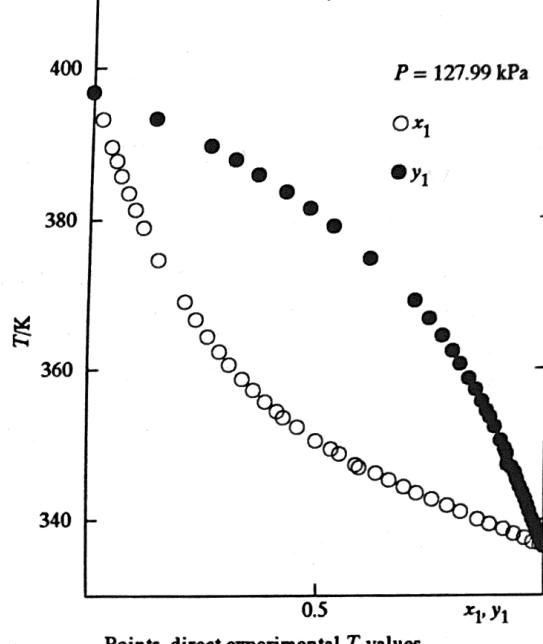
AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm^3 , ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer. High purity nitrogen was used for the backing pressure.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of $\pm 0.01\text{ K}$ with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa , indicated by an electronic pressure gauge (MKS Baratron).

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3593$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 926.99$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3974$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 805.93$.

Errors: $|8T(\text{estd.})|/K = 0.01$; $|8P(\text{estd.})|/\text{Pa} = 20$; $|8x_1| = 0.0005$ and 0.002 at 75 and 128 kPa; $|8y_1| = 0.002$ and 0.005 at 75 and 128 kPa.



REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Susial, P.; Ortega, J. J. Chem. Eng. Jpn. in press.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Components: 1. Methyl ethanoate, $C_3H_6O_2$ /79-20-9/
 2. 1-Butanol, $C_4H_{10}O$ /71-36-3/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

y_i , mole fraction of component i in vapor phase

x_i , mole fraction of component i in liquid phase

Parameters: P , pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P ; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

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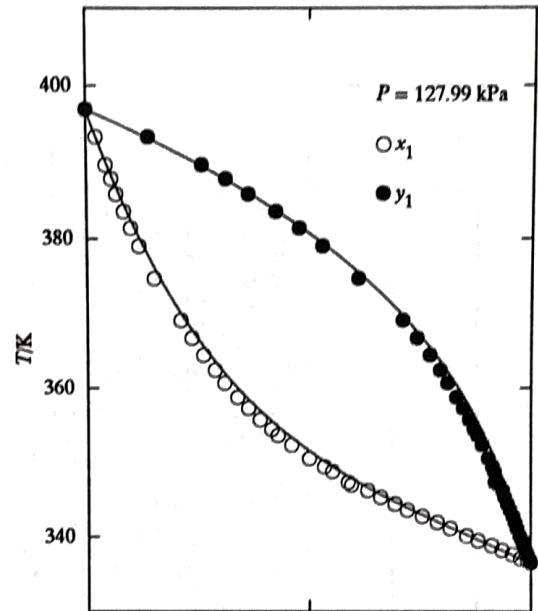
SOURCE OF DATA

Susial, P.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calcd. values of y_1

x_1	$P/kPa = 74.66$		$P/kPa = 127.99$				
	T/K	y_1	T/K	y_1			
0.00	381.87	0	397.02	0			
0.05	371.51	0.3607	388.65	0.2831			
0.10	362.82	0.5762	381.36	0.4766			
0.15	355.82	0.7045	375.11	0.6086			
0.20	350.26	0.7832	369.80	0.7000			
0.25	345.84	0.8337	365.30	0.7645			
0.30	342.28	0.8677	361.47	0.8113			
0.40	336.97	0.9095	355.37	0.8726			
0.50	333.19	0.9341	350.77	0.9100			
0.60	330.28	0.9508	347.15	0.9352			
0.70	327.85	0.9638	344.17	0.9540			
0.75	326.74	0.9697	342.83	0.9620			
0.80	325.65	0.9754	341.56	0.9696			
0.85	324.58	0.9811	340.33	0.9769			
0.90	323.49	0.9870	339.11	0.9842			
0.95	322.38	0.9932	337.88	0.9918			
1.00	321.21	1	336.60	1			

Std. dev. $\sigma(T)/K$, rel. std. dev. $100\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$
 at $P/kPa = 74.66$ are resp.: 0.043, 0.178, 0.094.
 at $P/kPa = 127.99$ are resp.: 0.099, 0.378, 0.285.



Points, direct experimental T values, curves, $T(x_1)$ and $T(y_1)$, calculated from the equations.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 74.66 and 127.99 kPa are reported in ref. 2.

Computations: The 43 T_{exp} data at 74.66 kPa and 40 T_{exp} data at 127.99 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i^0 (ref. 6).

Errors: Std. dev. $\sigma(T) = [\sum(T-T_{exp})^2/(N-n-2)]^{1/2}$,
 Rel. std. dev. $100\sigma(\delta P/P) = 100[\sum((P-P_{exp})/P_{exp})^2/(N-n-2)]^{1/2}$,
 N , no. of exp. points, ref. 2,
 n , no. of coefficients in the smoothing equation.

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T})/T \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T})/T \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y_i)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [A_i + B_i / (C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2
74.66	219.92 (4.1)	0 (0)	-437.67 (18.3)	174180 (7330)
127.99	279.32 (16.3)	0 (0)	-228.6 (46.8)	73625 (20300)

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parentheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
74.66	14.25797	-2662.78	-53.46	14.74871	-2882.42	-105.66
127.99	14.25642	-2662.78	-53.46	14.74507	-2882.42	-105.66

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 132.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1969, k-5550, 1976, k-5000, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsionopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Components: 1. Methyl propanoate, $C_4H_8O_2$ [554-12-1]
2. 1-Butanol, $C_4H_{10}O$ [71-36-3]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

x_i , mole fraction of component i in liquid phase

y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

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Susial, P.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 74.66$						$P/kPa = 101.32$											
x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1
0.0000	381.87	0.0000	0.4309	355.66	0.7793	0.0000	390.23	0.0000	0.4548	364.43	0.7680						
0.0061	381.14	0.0377	0.4601	354.71	0.7954	0.0044	389.92	0.0199	0.4816	363.65	0.7838						
0.0283	379.12	0.1335	0.4857	353.91	0.8095	0.0182	388.56	0.0787	0.5235	362.46	0.8049						
0.0411	377.71	0.1824	0.5273	352.84	0.8272	0.0280	387.65	0.1168	0.5548	361.66	0.8205						
0.0524	376.72	0.2216	0.5576	352.04	0.8411	0.0513	385.67	0.1920	0.5861	360.90	0.8338						
0.0684	375.24	0.2774	0.5890	351.29	0.8536	0.0662	384.45	0.2382	0.6165	360.07	0.8486						
0.0827	374.04	0.3203	0.6211	350.53	0.8651	0.0799	383.38	0.2780	0.6483	359.35	0.8611						
0.1169	371.27	0.4115	0.6340	350.25	0.8706	0.0969	381.96	0.3231	0.6779	358.68	0.8732						
0.1290	370.09	0.4377	0.6662	349.56	0.8824	0.1263	380.12	0.3888	0.7092	358.01	0.8862						
0.1519	368.70	0.4897	0.7000	348.83	0.8943	0.1480	378.62	0.4367	0.7379	357.38	0.8968						
0.1715	367.34	0.5226	0.7339	348.13	0.9057	0.1725	376.88	0.4802	0.7716	356.69	0.9098						
0.1960	365.94	0.5614	0.7650	347.55	0.9166	0.1898	375.86	0.5104	0.8012	356.10	0.9214						
0.2195	364.55	0.5962	0.7986	346.91	0.9280	0.2146	374.56	0.5478	0.8376	355.32	0.9349						
0.2406	363.42	0.6223	0.8303	346.31	0.9388	0.2297	373.62	0.5678	0.8656	354.77	0.9457						
0.2440	363.19	0.6277	0.8597	345.77	0.9491	0.2598	372.18	0.6048	0.8931	354.23	0.9563						
0.2734	361.65	0.6613	0.8901	345.20	0.9595	0.2846	371.09	0.6337	0.9150	353.80	0.9655						
0.2865	361.23	0.6731	0.9211	344.56	0.9704	0.3097	369.90	0.6589	0.9385	353.32	0.9746						
0.3088	360.22	0.6929	0.9488	344.02	0.9807	0.3440	368.45	0.6882	0.9560	352.99	0.9818						
0.3316	359.06	0.7123	0.9707	343.60	0.9887	0.3737	367.35	0.7128	0.9738	352.66	0.9893						
0.3530	358.20	0.7306	0.9866	343.31	0.9947	0.3972	366.53	0.7304	0.9872	352.41	0.9948						
0.3983	356.71	0.7584	1.0000	343.05	1.0000	0.4283	365.30	0.7531	1.0000	352.16	1.0000						

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

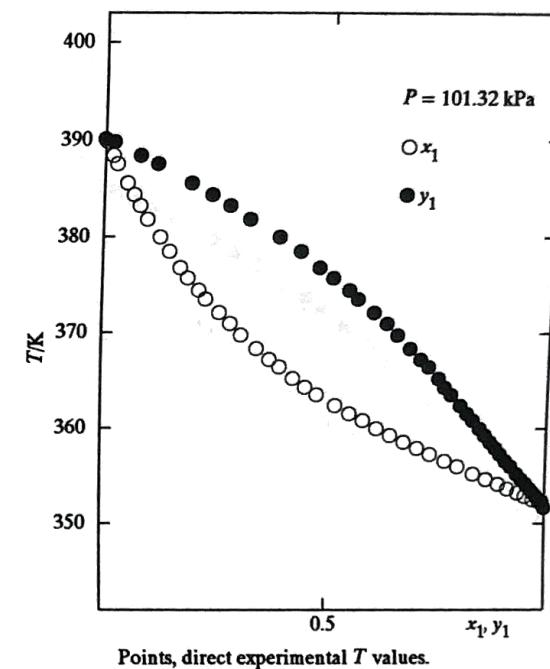
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ± 0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3740$, $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^3 = 908.53$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3974$, $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^3 = 805.93$.

Errors: $|\delta T(\text{estd.})|/K = 0.01$; $|\delta P(\text{estd.})|/\text{Pa} = 30$; $|\delta x_1| = 0.001$; $|\delta y_1| = 0.001$ and 0.006 at 75 and 101 kPa.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Susial, P.; Ortega, J. J. Chem. Eng. Data 1993, 38, 647.
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Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain)

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DIRECT EXPERIMENTAL VALUES

$P/kPa = 127.99$

x_1	T/K	y_1	x_1	T/K	y_1
0.0000	397.02	0.0000	0.4887	371.57	0.7682
0.0048	396.48	0.0228	0.5248	370.37	0.7892
0.0117	395.89	0.0488	0.5609	369.29	0.8083
0.0201	395.28	0.0745	0.5908	368.39	0.8232
0.0332	394.24	0.1188	0.6311	367.36	0.8435
0.0436	393.39	0.1523	0.6588	366.69	0.8556
0.0597	392.24	0.1989	0.6878	365.99	0.8693
0.0788	390.90	0.2482	0.7266	365.13	0.8856
0.0963	389.63	0.2926	0.7636	364.39	0.9009
0.1169	388.26	0.3415	0.7941	363.67	0.9137
0.1519	386.04	0.4142	0.8286	362.85	0.9280
0.1766	384.59	0.4555	0.8635	362.03	0.9423
0.1976	383.30	0.4901	0.8939	361.34	0.9547
0.2335	381.45	0.5445	0.9196	360.80	0.9656
0.2762	379.47	0.5954	0.9416	360.34	0.9747
0.3033	378.41	0.6230	0.9566	360.05	0.9814
0.3294	377.24	0.6499	0.9720	359.75	0.9879
0.3645	375.86	0.6820	0.9863	359.48	0.9941
0.4241	373.70	0.7264	1.0000	359.22	1.0000
0.4524	372.56	0.7478			

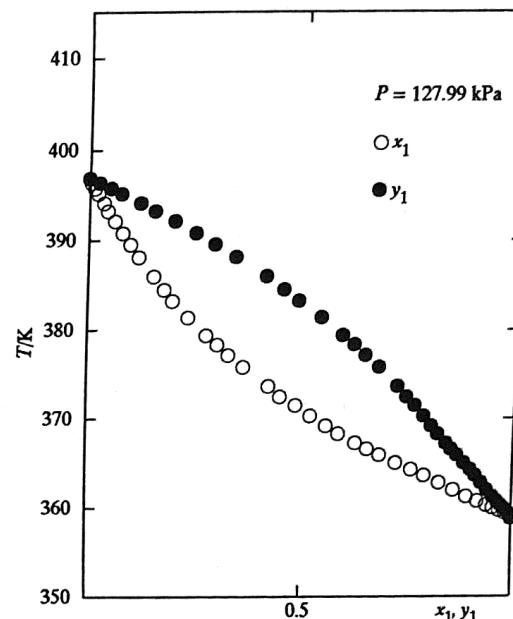
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Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3740$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 908.53$.
 2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3974$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 805.93$.

Errors: $|\delta T(\text{estd.})|/K = 0.01$; $|\delta P(\text{estd.})|/\text{Pa} = 30$; $|\delta x_1| = 0.002$; $|\delta y_1| = 0.007$.



Points, direct experimental T values.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Susial, P.; Ortega, J. J. Chem. Eng. Data 1993, 38, 647.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Components: 1. Methyl propanoate, $C_4H_8O_2$ [554-12-1]
2. 1-Butanol, $C_4H_{10}O$ [71-36-3]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

y_i , mole fraction of component i in vapor phase

x_i , mole fraction of component i in liquid phase

Parameters: P , pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P ; ref. 1

Author(s) of table 3k: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

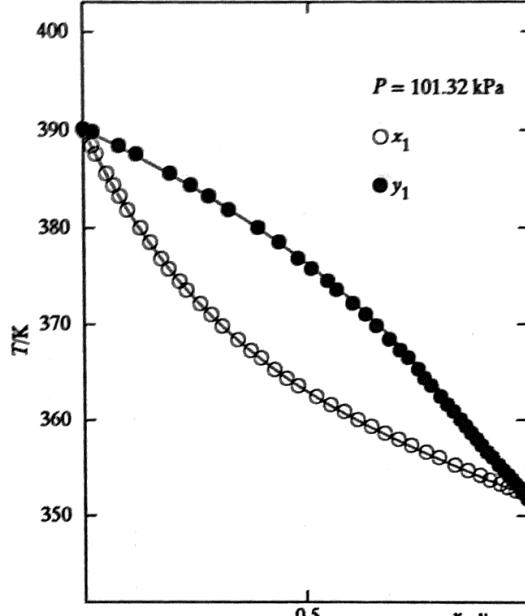
SOURCE OF DATA

Susial, P.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calcd. values of y_1

	$P/kPa = 74.66$		$P/kPa = 101.32$		$P/kPa = 127.99$		
x_1	T/K	y_1	T/K	y_1	T/K	y_1	
0.00	381.87	0	390.23	0	397.02	0	
0.05	376.96	0.2086	385.75	0.1875	392.98	0.1688	
0.10	372.63	0.3643	381.82	0.3311	389.38	0.3028	
0.15	368.87	0.4805	378.37	0.4422	386.16	0.4100	
0.20	365.64	0.5680	375.35	0.5295	383.29	0.4967	
0.25	362.87	0.6351	372.69	0.5991	380.71	0.5676	
0.30	360.48	0.6876	370.33	0.6555	378.40	0.6264	
0.40	356.61	0.7643	366.37	0.7410	374.42	0.7178	
0.50	353.56	0.8186	363.16	0.8029	371.11	0.7859	
0.60	351.05	0.8610	360.48	0.8510	368.27	0.8397	
0.70	348.86	0.8973	358.16	0.8911	365.76	0.8846	
0.75	347.84	0.9143	357.09	0.9095	364.60	0.9050	
0.80	346.85	0.9309	356.07	0.9272	363.48	0.9245	
0.85	345.88	0.9476	355.07	0.9447	362.39	0.9434	
0.90	344.93	0.9645	354.10	0.9624	361.32	0.9621	
0.95	343.99	0.9818	353.13	0.9807	360.27	0.9809	
1.00	343.05	1	352.16	1	359.22	1	

Std. dev. $\sigma(T)/K$, rel. std. dev. $100\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$
at $P/kPa = 74.66$ are resp.: 0.066, 0.255, 1.162.
at $P/kPa = 101.32$ are resp.: 0.053, 0.195, 0.148.
at $P/kPa = 127.99$ are resp.: 0.075, 0.256, 0.137.



Points, direct experimental T values, curves, $T(x_1)$ and $T(y_1)$, calculated from the equations.

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T}) \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T}) \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1 - y_i)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [A_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2
74.66	200.05 (5.3)	0 (0)	38.033 (4.1)	0 (0)
101.32	207.15 (4.9)	0 (0)	14.6 (3.7)	0 (0)
127.99	163.43 (8.1)	0 (0)	20.877 (6.6)	0 (0)

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parantheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
74.66	13.80054	-2600.93	-68.91	15.33484	-3212.43	-90.41
101.32	13.80074	-2600.93	-68.91	15.33285	-3212.43	-90.41
127.99	13.8111	-2600.93	-68.91	15.32924	-3212.43	-90.41

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 134, 135.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1969, k-5580, 1976, k-5000, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsonopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 74.66, 101.32 and 127.99 kPa are reported in ref. 2.

Computations: The 42 T_{exp} data at 74.66 kPa, 42 T_{exp} data at 101.32 kPa and 39 T_{exp} data at 127.99 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i^0 (ref. 6).

Errors: Std. dev. $\sigma(T) = [\sum(T - T_{exp})^2/(N-n-2)]^{1/2}$,
Rel. std. dev. $100\sigma(\delta P/P) = 100[\sum((P - P_{exp})/P_{exp})^2/(N-n-2)]^{1/2}$,
 N , no. of exp. points, ref. 2,
 n , no. of coefficients in the smoothing equation.

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Components: 1. Ethyl ethanoate, $C_4H_8O_2$ [141-78-6]
 2. 1-Butanol, $C_4H_{10}O$ [71-36-3]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

x_i , mole fraction of component i in liquid phase

y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$

x_1	T/K	y_1	x_1	T/K	y_1							
0.0000	390.90	0.0000	0.4901	361.65	0.8033							
0.0408	386.85	0.1615	0.5422	360.15	0.8299							
0.0624	384.75	0.2316	0.5881	358.95	0.8499							
0.0948	381.75	0.3286	0.6113	358.15	0.8589							
0.1167	380.05	0.3826	0.6436	357.75	0.8713							
0.1383	378.45	0.4303	0.6937	356.15	0.8910							
0.1524	377.45	0.4609	0.7201	355.95	0.8999							
0.1803	375.45	0.5174	0.7524	355.25	0.9122							
0.1931	374.65	0.5369	0.7923	354.35	0.9277							
0.2423	371.55	0.6022	0.8367	353.05	0.9436							
0.2753	369.85	0.6422	0.8692	352.85	0.9540							
0.3348	367.15	0.7032	0.9191	351.75	0.9714							
0.3721	365.65	0.7328	0.9590	351.15	0.9874							
0.4133	364.05	0.7618	1.0000	350.30	1.0000							
0.4455	362.95	0.7785										

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm^3 , ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of $\pm 0.1\text{ K}$ with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa .

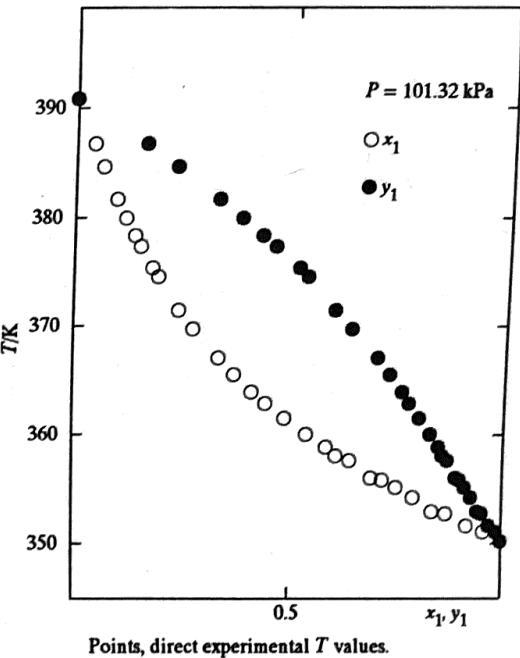
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3699$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 894.34$.

2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3974$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 805.73$.

Errors: $|\delta T(\text{estd.})|/K = 0.1$; $|\delta P(\text{estd.})|/\text{Pa} = 70$; $|\delta x_1| = 0.001$; $|\delta y_1| = 0.01$.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Pena, J. A.; de Alfonso, C. Rev. Latinoamer. Ing. Quim. Apl. 1986, 13, 317.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.



Components: 1. Ethyl ethanoate, $C_4H_8O_2$ /141-78-6/
2. 1-Butanol, $C_4H_{10}O$ /71-36-3/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

y_i , mole fraction of component i in vapor phase

x_i , mole fraction of component i in liquid phase

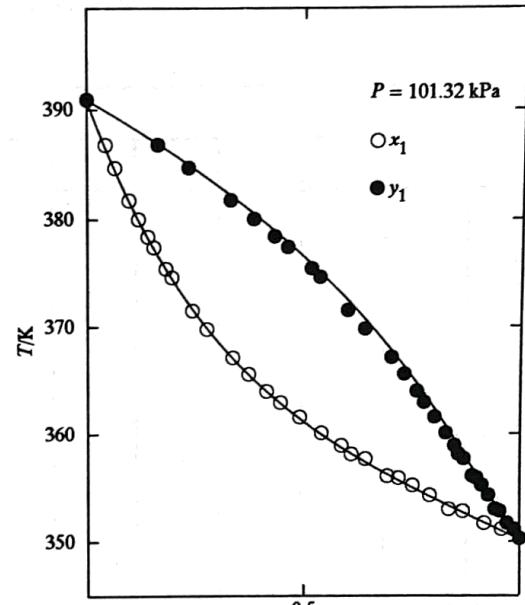
Parameters: P , pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P ; ref. 1

Notes: The table reports smoothed values of T and calcd. values of y_1

x_1	T/K	y_1					
0.00	390.90	0					
0.05	386.01	0.1982					
0.10	381.54	0.3513					
0.15	377.58	0.4676					
0.20	374.15	0.5557					
0.25	371.20	0.6233					
0.30	368.67	0.6763					
0.40	364.54	0.7538					
0.50	361.31	0.8090					
0.60	358.63	0.8526					
0.70	356.30	0.8902					
0.75	355.22	0.9080					
0.80	354.18	0.9255					
0.85	353.18	0.9432					
0.90	352.20	0.9612					
0.95	351.24	0.9800					
1.00	350.30	1					

Std. dev. $\sigma(T)/K$, rel. std. dev. $100\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$ at $P/kPa = 101.32$ are resp.: 0.122, 0.435, 0.351.



Points, direct experimental T values, curves, $T(x_1)$ and $T(y_1)$, calculated from the equations.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.

Computations: The 29 T_{exp} data at 101.32 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i^0 (ref. 6).

Errors: Std. dev. $\sigma(T) = [\sum(T - T_{exp})^2/(N-n-2)]^{1/2}$,
Rel. std. dev. $100\sigma(\delta P/P) = 100[\sum((P - P_{exp})/P_{exp})^2/(N-n-2)]^{1/2}$,
 n , no. of exp. points, ref. 2,
 n , no. of coefficients in the smoothing equation.

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain)

Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Pena, J.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T})/T \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T})/T \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [A_i + B_i / (C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2	
101.32	250.61 (10.9)	0 (0)	2.229 (7.5)	0 (0)	

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parentheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
101.33	14.12011	-2751.89	-60.68	15.30906	-3212.43	-90.41

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 137.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1969, k-5550, 1976, k-5000, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsionopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Components: 1. 1-Butanol, $C_4H_{10}O$ /71-36-3/
 2. Ethyl propanoate, $C_5H_{10}O_2$ /105-37-3/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

x_i , mole fraction of component i in liquid phase

y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain)

Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$

x_1	T/K	y_1	x_1	T/K	y_1															
0.1427	372.70	0.0927	0.6028	378.30	0.4279															
0.1849	373.00	0.1218	0.6296	378.80	0.4498															
0.2260	373.30	0.1414	0.6575	379.30	0.4725															
0.2648	373.70	0.1812	0.6816	379.80	0.4947															
0.2944	374.00	0.2015	0.7037	380.0	0.5173															
0.3229	374.30	0.2226	0.7323	381.00	0.5468															
0.3502	374.60	0.2419	0.7569	381.50	0.5745															
0.3731	374.90	0.2578	0.7821	382.10	0.6031															
0.3966	375.20	0.2764	0.8006	382.60	0.6253															
0.4391	375.70	0.3073	0.8264	383.30	0.6572															
0.4482	375.90	0.3146	0.8501	383.90	0.6902															
0.4778	376.30	0.3351	0.8658	384.40	0.7124															
0.5175	376.90	0.3638	0.8951	385.40	0.7595															
0.5500	377.40	0.3869	0.9099	385.90	0.7840															
0.5701	377.70	0.4016	0.9274	386.60	0.8176															

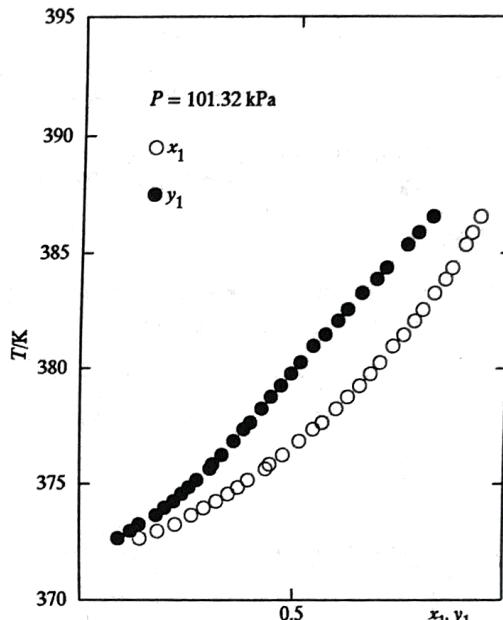
AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm^3 , ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of $\pm 0.1\text{ K}$ with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa .

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 805.73$.
 2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss" grade material, purity > 99.0 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 883.91$.

Errors: $|\delta T(\text{estd.})|/K = 0.1$; $|\delta P(\text{estd.})|/\text{Pa} = 70$; $|\delta x_1| = 0.001$; $|\delta y_1| = 0.01$.



Points, direct experimental T values.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. Can. J. Chem. Eng. 1987, 65, 982.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Components: 1. 1-Butanol, $C_4H_{10}O$ [71-36-3]
2. Ethyl propanoate, $C_5H_{10}O_2$ [105-37-3]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

y_i , mole fraction of component i in vapor phase

x_i , mole fraction of component i in liquid phase

Parameters: P , pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P ; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

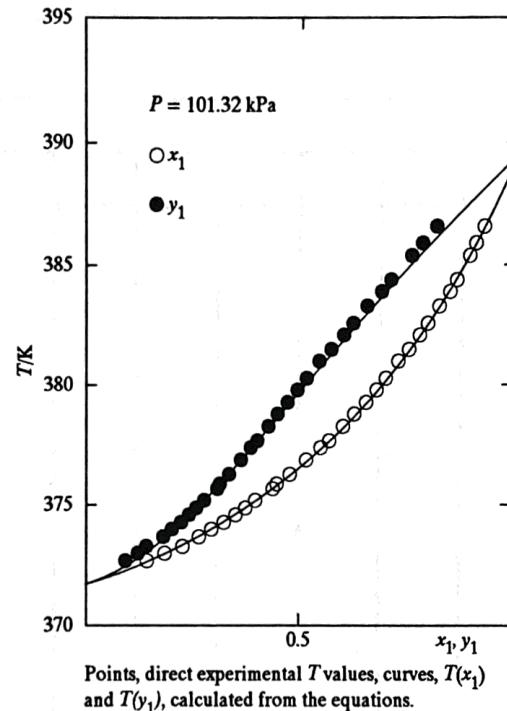
SOURCE OF DATA

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Notes: The table reports smoothed values of T and calcd. values of y_1

x_1	T/K	y_1					
0.00	371.80	0					
0.05	372.06	0.0413					
0.10	372.38	0.0792					
0.15	372.75	0.1146					
0.20	373.16	0.1484					
0.25	373.61	0.1811					
0.30	374.11	0.2132					
0.40	375.24	0.2782					
0.50	376.58	0.3473					
0.60	378.20	0.4253					
0.70	380.16	0.5183					
0.75	381.31	0.5730					
0.80	382.59	0.6349					
0.85	384.02	0.7060					
0.90	385.64	0.7885					
0.95	387.45	0.8853					
1.00	389.50	1					

Std. dev. $\sigma(T)/K$, rel. std. dev. 100 $\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$ at $P/kPa = 101.32$ are resp.: 0.054, 0.19, 0.111.



AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2

Computations: The 32 T_{exp} data at 101.32 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i^0 (ref. 6).

Errors: Std. dev. $\sigma(T) = [\sum(T-T_{exp})^2/(N-n)]^{1/2}$,
Rel. std. dev. 100 $\sigma(\delta P/P) = 100[\sum((P-P_{exp})/P_{exp})^2/(N-n)]^{1/2}$,
 N , no. of exp. points, ref. 2,
 n , no. of coefficients in the smoothing equation.

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp\left[-(a_1 + \frac{a_2}{T})\right] \quad c_2 = \exp\left[-(a_3 + \frac{a_4}{T})\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp\left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y_i)^2}{RT}\right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp[A_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2
101.32	46.766 (6)	0 (0)	153.96 (7)	0 (0)

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parentheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
101.32	15.359	-3212.43	-90.41	14.1587	-2935.11	-64.15

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 139.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1969, k-5580, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsonopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Components: 1. 1-Butanol, $C_4H_{10}O$ [71-36-3]
 2. Ethyl butanoate, $C_6H_{12}O_2$ [105-54-4]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

x_i , mole fraction of component i in liquid phase

y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$

x_1	T/K	y_1	x_1	T/K	y_1															
0.0339	392.80	0.0625	0.4960	388.40	0.5150															
0.0427	392.60	0.0750	0.5216	388.30	0.5355															
0.0561	392.40	0.0932	0.5468	388.30	0.5556															
0.0766	392.10	0.1209	0.5666	388.30	0.5707															
0.0919	391.80	0.1396	0.6162	388.30	0.6110															
0.1245	391.20	0.1796	0.6367	388.40	0.6269															
0.1707	390.50	0.2308	0.6534	388.40	0.6411															
0.2127	390.00	0.2747	0.6783	388.50	0.6620															
0.2578	389.60	0.3190	0.6934	388.50	0.6743															
0.2911	389.30	0.3498	0.7263	388.60	0.7024															
0.3058	389.30	0.3618	0.7664	388.80	0.7370															
0.3456	389.00	0.3952	0.7932	388.90	0.7615															
0.3638	388.90	0.4099	0.8209	389.00	0.7876															
0.3852	388.80	0.4273	0.8653	389.30	0.8316															
0.4030	388.70	0.4412	0.9035	389.60	0.8723															
0.4398	388.60	0.4715	0.9308	389.80	0.9019															
0.4557	388.50	0.4840	0.9679	390.20	0.9455															
0.4847	388.40	0.5065	0.9843	390.30	0.9685															

AUXILIARY INFORMATION

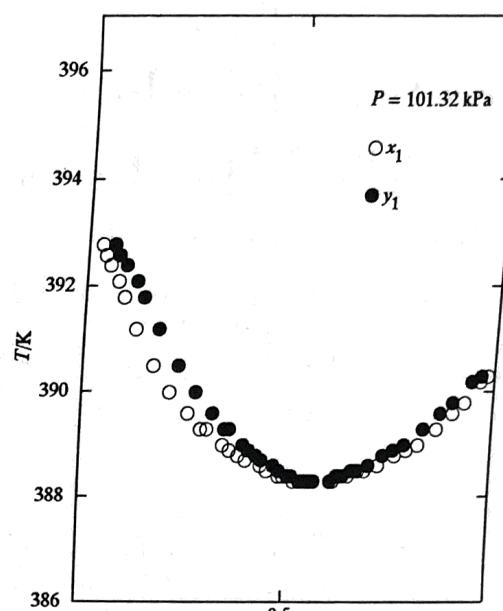
Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ± 0.1 K with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 799.54$.

2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mole %, treated with calcium chloride, dried with potassium carbonate, and fractionally distd. through a 120-plate lab. column; degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 873.75$.

Errors: $|\delta T(\text{estd.})|/K = 0.1$; $|\delta P(\text{estd.})|/\text{Pa} = 70$; $|\delta x_1| = 0.0002$; $|\delta y_1| = 0.004$.



Points, direct experimental T values.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Pena, J. A.; de Alfonso, C. Rev. Latinoamer. Ing. Quim. Apl. 1987, 17, 195.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Components: 1. 1-Butanol, C₄H₁₀O /71-36-3/
 2. Ethyl butanoate, C₆H₁₂O₂ /105-54-4/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T, temperature

y_i, mole fraction of component i in vapor phase

x_i, mole fraction of component i in liquid phase

Parameters: P, pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp}, data at variable x_i and constant P; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

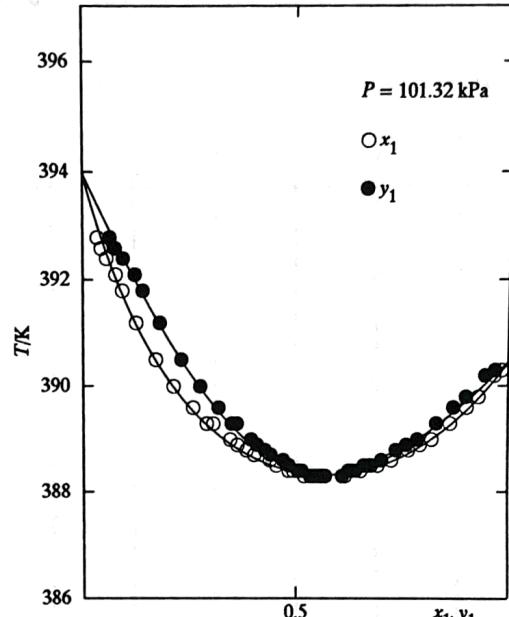
SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calcd. values of y_i

x ₁	T/K	y ₁					
0.00	394.00	0					
0.05	392.66	0.0809					
0.10	391.61	0.1493					
0.15	390.79	0.2088					
0.20	390.14	0.2617					
0.25	389.63	0.3098					
0.30	389.23	0.3545					
0.40	388.68	0.4370					
0.50	388.41	0.5154					
0.60	388.36	0.5941					
0.70	388.53	0.6773					
0.75	388.70	0.7219					
0.80	388.92	0.7692					
0.85	389.21	0.8199					
0.90	389.56	0.8747					
0.95	389.99	0.9344					
1.00	390.50	1					

Std. dev. σ(T)/K, rel. std. dev. 100σ(δP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.320 are resp.: 0.07, 0.202, 0.056.



Points, direct experimental T values, curves, T(x₁) and T(y₁), calculated from the equations.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.320 kPa are reported in ref. 2.

Computations: The 36 T_{exp} data at 101.320 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E.

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i⁰ (ref. 6).

Errors: Std. dev. σ(T) = [Σ(T-T_{exp})²/(N-n)]^{1/2},
 Rel. std. dev. 100σ(δP/P) = 100[Σ((P-P_{exp})/P_{exp})²/(N-n)]^{1/2},
 N, no. of exp. points, ref. 2,
 n, no. of coefficients in the smoothing equation.

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T}) \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T}) \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y_i)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [A_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.320	53.52 (4.2)	0 (0)	139.88 (4.4)	0 (0)

The std. deviations σ(a_i) of the coeffs. a_i are given in parentheses.

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.73786	-2882.42	-105.66	12.1636	-2121.97	-112.77

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 141.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1978, k-5620, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsionopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Components:	1. 1-Butanol, C ₄ H ₁₀ O /71-36-3/ 2. Propyl ethanoate, C ₅ H ₁₀ O ₂ /109-60-4/
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	T, temperature x_i , mole fraction of component <i>i</i> in liquid phase y_i , mole fraction of component <i>i</i> in vapor phase
Parameters:	P, pressure
Method:	Direct measurement of T, x_i , and y_i at constant P; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

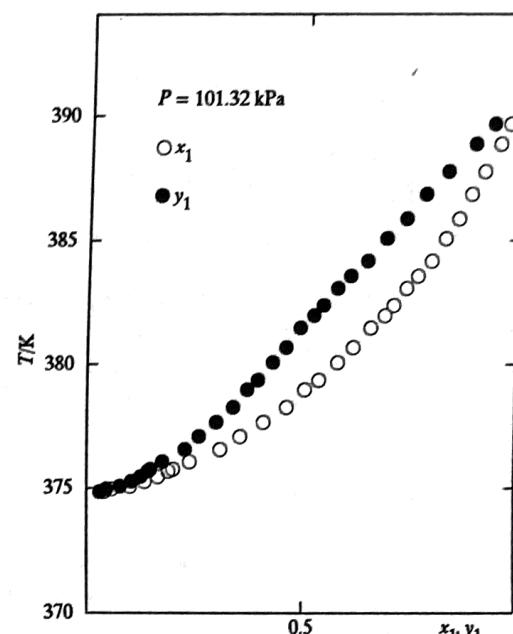
Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$					
x_1	T/K	y_1	x_1	T/K	y_1
0.0416	374.90	0.0328	0.5830	380.10	0.4325
0.0601	375.00	0.0477	0.6192	380.70	0.4624
0.1028	375.10	0.0794	0.6587	381.50	0.4959
0.1371	375.30	0.1061	0.6905	382.00	0.5267
0.1675	375.50	0.1281	0.7113	382.40	0.5477
0.1925	375.70	0.1448	0.7403	383.10	0.5805
0.2037	375.80	0.1511	0.7654	383.60	0.6094
0.2411	376.10	0.1777	0.7964	384.20	0.6475
0.3118	376.60	0.2304	0.8272	385.10	0.6906
0.3592	377.10	0.2636	0.8566	385.90	0.7358
0.4128	377.70	0.3038	0.8842	386.90	0.7789
0.4663	378.30	0.3420	0.9146	387.80	0.8290
0.5084	379.00	0.3740	0.9487	388.90	0.8902
0.5394	379.40	0.3990	0.9700	389.70	0.9333



Points, direct experimental T values.

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ± 0.1 K with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 805.73$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 95 mole %, washed with sodium carbonate, treated with calcium chloride, dried with potassium carbonate, and fractionally, distd. through a 120-plate lab. column; degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 880.97$.

Errors: $|\delta T(\text{estd.})|/K = 0.1$; $|\delta P(\text{estd.})|/Pa = 70$; $|\delta x_1| = 0.0005$; $|\delta y_1| = 0.008$.

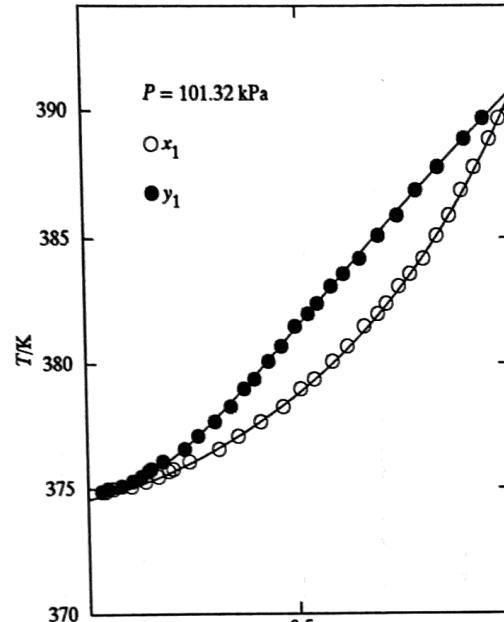
REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. Can. J. Chem. Eng. 1987, 65, 982.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Components:	1. 1-Butanol, C ₄ H ₁₀ O [71-36-3] 2. Propyl ethanoate, C ₅ H ₁₀ O ₂ [109-60-4]	Author(s) of table 3k: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor	Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)
Variables:	T, temperature	
	y _i , mole fraction of component i in vapor phase	
Parameters:	x _i , mole fraction of component i in liquid phase	
Method:	P, pressure	SOURCE OF DATA
	Calculation from direct experimental liquid-vapor equilibrium temperature, T _{exp} , data at variable x _i and constant P; ref. 1	Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calcd. values of y₁

x ₁	T/K	y ₁					
0.00	374.64	0					
0.05	374.82	0.0436					
0.10	375.07	0.0834					
0.15	375.38	0.1205					
0.20	375.73	0.1556					
0.25	376.13	0.1895					
0.30	376.58	0.2228					
0.40	377.61	0.2896					
0.50	378.85	0.3601					
0.60	380.35	0.4391					
0.70	382.18	0.5323					
0.75	383.25	0.5866					
0.80	384.44	0.6477					
0.85	385.78	0.7173					
0.90	387.28	0.7974					
0.95	388.96	0.8906					
1.00	390.85	1					

Std. dev. σ(T)/K, rel. std. dev. 100σ(dP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.065, 0.221, 0.141.Points, direct experimental T values, curves, T(x₁) and T(y₁), calculated from the equations.

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T}) \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T}) \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y_i)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [A_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²	
101.32	42.605 (8)	0 (0)	158.8 (9.4)	0 (0)	

The std. deviations σ(a_i) of the coeffs. a_i are given in parentheses.

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	15.31058	-3212.43	-90.41	13.94327	-2840.15	-70.07

REFERENCES

- Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
- Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 143.
- Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
- TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1969, k-5550, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
- Tsonopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
- Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.Computations: The 28 T_{exp} data at 101.32 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E.Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i⁰ (ref. 6).Errors: Std. dev. σ(T) = [Σ(T-T_{exp})²/(N-n)]^{1/2},
Rel. std. dev. 100σ(dP/P) = 100[Σ((P-P_{exp})/P_{exp})²/(N-n)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. of coefficients in the smoothing equation.

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Components: 1. 1-Butanol, $C_4H_{10}O$ /71-36-3/
2. Propyl propanoate, $C_6H_{12}O_2$ /106-36-5/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

x_i , mole fraction of component i in liquid phase

y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Direct measurement of T , x_i , and y_i at constant P ; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES $P/kPa = 101.32$

x_1	T/K	y_1	x_1	T/K	y_1															
0.0000	395.65	0.0000	0.5471	389.47	0.5793															
0.0348	394.91	0.0552	0.5810	389.40	0.6054															
0.1006	393.61	0.1486	0.6057	389.35	0.6208															
0.1242	393.32	0.1754	0.6354	389.33	0.6447															
0.1530	392.83	0.2106	0.6710	389.26	0.6735															
0.2106	392.01	0.2751	0.6958	389.27	0.6887															
0.2214	391.87	0.2877	0.7196	389.27	0.7095															
0.2380	391.69	0.3061	0.7511	389.35	0.7353															
0.2590	391.41	0.3274	0.8428	389.63	0.8211															
0.2839	391.11	0.3517	0.8710	389.81	0.8493															
0.3209	390.78	0.3871	0.8949	389.96	0.8747															
0.3479	390.56	0.4122	0.9156	390.12	0.8980															
0.3685	390.37	0.4302	0.9330	390.22	0.9174															
0.4179	390.05	0.4718	0.9502	390.37	0.9371															
0.4385	389.93	0.4858	0.9779	390.60	0.9710															
0.4603	389.79	0.5064	0.9884	390.74	0.9834															
0.4895	389.67	0.5297	1.0000	390.85	1.0000															
0.5206	389.56	0.5545																		

AUXILIARY INFORMATION

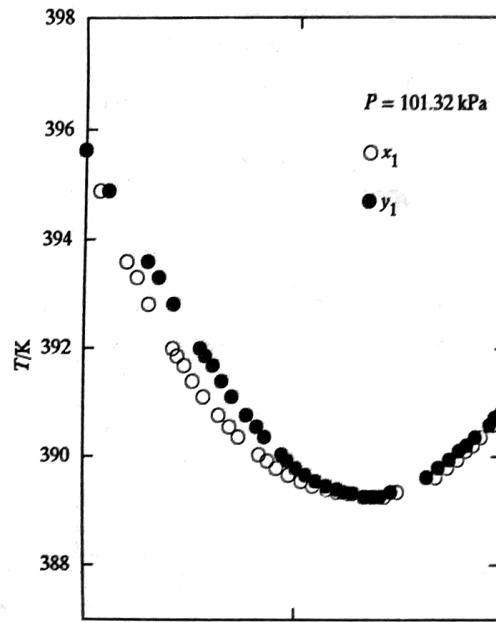
Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ± 0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter having a precision of ± 0.02 kg·m⁻³. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.8 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3974$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 805.93$.

2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15\text{ K}) = 1.3918$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 875.65$.

Errors: $|\delta T(\text{estd.})|/K = 0.01$; $|\delta P(\text{estd.})|/Pa = 20$; $|\delta x_1| = 0.0005$; $|\delta y_1| = 0.003$.



Points, direct experimental T values.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Galvan, S. J. Chem. Eng. Data 1944, 39, 907.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Published by Thermodynamics Research Center

Components: 1. 1-Butanol, $C_4H_{10}O$ /71-36-3/2. Propyl propanoate, $C_6H_{12}O_2$ /106-36-5/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature y_i , mole fraction of component i in vapor phase x_i , mole fraction of component i in liquid phaseParameters: P , pressureMethod: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P ; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., of table 3k: Canary Islands, Spain)

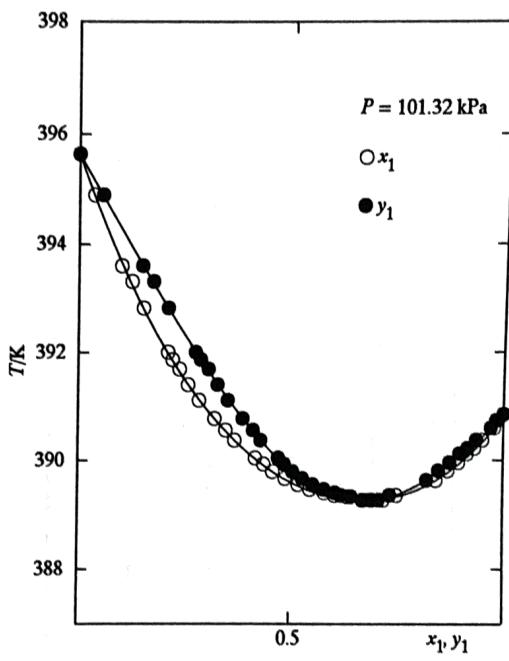
Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calcd. values of y_1

x_1	T/K	y_1				
0.00	395.65	0				
0.05	394.61	0.0767				
0.10	393.68	0.1461				
0.15	392.86	0.2091				
0.20	392.14	0.2667				
0.25	391.52	0.3195				
0.30	390.99	0.3684				
0.40	390.17	0.4572				
0.50	389.63	0.5381				
0.60	389.33	0.6155				
0.70	389.28	0.6943				
0.75	389.35	0.7357				
0.80	389.49	0.7796				
0.85	389.70	0.8269				
0.90	389.99	0.8785				
0.95	390.37	0.9358				
1.00	390.85	1				

Std. dev. $\sigma(T)/K$, rel. std. dev. $100\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$ at $P/kPa = 101.320$ are resp.: 0.022, 0.07, 0.051.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.320 kPa are reported in ref. 2.Computations: The 35 T_{exp} data at 101.320 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E .Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data.Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i^0 (ref. 6).Errors: Std. dev. $\sigma(T) = [\sum(T-T_{exp})^2/(N-n-2)]^{1/2}$,Rel. std. dev. $100\sigma(\delta P/P) = 100[\sum((P-P_{exp})/P_{exp})^2/(N-n-2)]^{1/2}$, N , no. of exp. points, ref. 2, n , no. of coefficients in the smoothing equation.

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T})/T \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T})/T \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [4a_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2	
101.320	-2015.51 (183)	855370 (69500)	13.201 (4.9)	0 (0)	

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parentheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
101.32	15.31074	-3212.43	-90.41	14.84882	-3558.18	-47.85

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 145.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1969, k-5580, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsionopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Components: 1. 1-Butanol, C₄H₁₀O /11-36-3/
 2. Propyl butanoate, C₇H₁₄O₂ /105-66-8/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T, temperature

x_i, mole fraction of component i in liquid phase

y_i, mole fraction of component i in vapor phase

Parameters: P, pressure

Method: Direct measurement of T, x_i, and y_i at constant P; ref. 1

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., of table: Canary Islands, Spain)

Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32

x ₁	T/K	y ₁	x ₁	T/K	y ₁							
0.0000	416.65	0.0000	0.5117	396.60	0.6952							
0.0863	411.15	0.1908	0.5437	396.30	0.7063							
0.1171	409.03	0.2614	0.5710	395.75	0.7175							
0.1486	407.47	0.3237	0.5969	395.29	0.7383							
0.1821	406.05	0.3698	0.6281	394.85	0.7567							
0.2235	403.98	0.4313	0.6645	394.38	0.7743							
0.2490	403.05	0.4664	0.6930	393.90	0.7928							
0.2705	402.55	0.4897	0.7283	393.37	0.8152							
0.3166	401.45	0.5303	0.7575	392.92	0.8354							
0.3538	400.15	0.5723	0.7829	392.56	0.8537							
0.3890	399.45	0.5988	0.8080	392.25	0.8710							
0.4267	398.82	0.6185	0.8700	391.59	0.9081							
0.4587	397.95	0.6485	0.9378	390.93	0.9540							
0.4844	397.28	0.6712	1.0000	390.23	1.0000							

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).

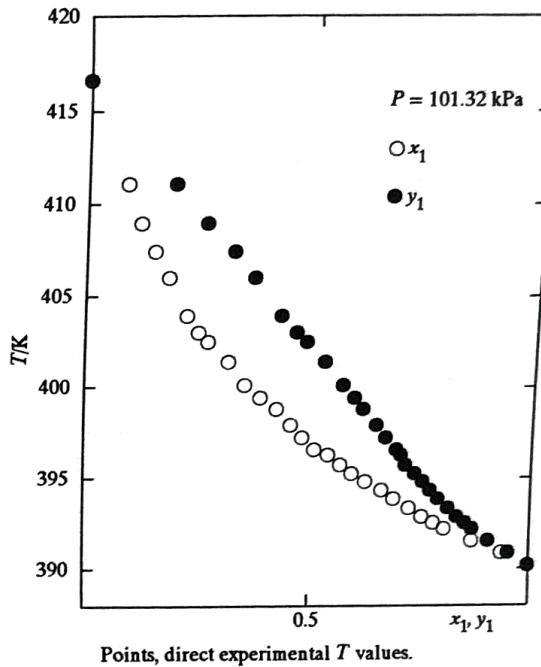
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.8 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); n(D, 298.15 K) = 1.3974, ρ(298.15 K)/kg·m⁻³ = 805.93.

2. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); n(D, 298.15 K) = 1.3976, ρ(298.15 K)/kg·m⁻³ = 868.07.

Errors: |δT(estd.)|/K = 0.01; |δP(estd.)|/Pa = 20; |δx₁| = 0.005; |δy₁| = 0.01.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Galvan, S. J. Chem. Eng. Data in press.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.



Points, direct experimental T values.

Components: 1. 1-Butanol, $C_4H_{10}O$ /71-36-3/
2. Propyl butanoate, $C_7H_{14}O_2$ /105-66-8/

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature

y_i , mole fraction of component i in vapor phase

x_i , mole fraction of component i in liquid phase

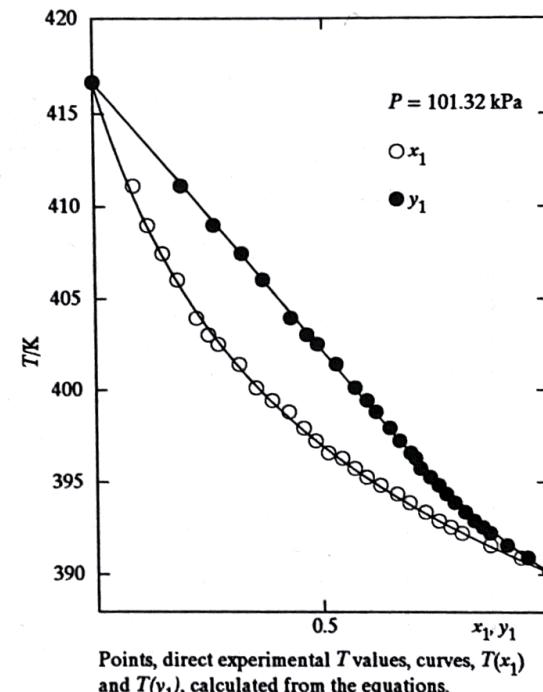
Parameters: P , pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P ; ref. 1

Notes: The table reports smoothed values of T and calcd. values of y_1

x_1	T/K	y_1					
0.00	416.65	0					
0.05	412.89	0.1347					
0.10	409.86	0.2403					
0.15	407.34	0.3262					
0.20	405.22	0.3980					
0.25	403.39	0.4595					
0.30	401.80	0.5133					
0.40	399.16	0.6043					
0.50	397.02	0.6809					
0.60	395.25	0.7488					
0.70	393.74	0.8119					
0.75	393.06	0.8426					
0.80	392.42	0.8732					
0.85	391.82	0.9040					
0.90	391.26	0.9351					
0.95	390.73	0.9671					
1.00	390.23	1					

Std. dev. $\sigma(T)/K$, rel. std. dev. $100\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$ at $P/kPa = 101.32$ kPa are resp.: 0.178, 0.524, 0.503.



Points, direct experimental T values, curves, $T(x_1)$ and $T(y_1)$, calculated from the equations.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.

Computations: The 28 T_{exp} data at 101.32 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess Gibbs energies μ_i^E .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental VLE data. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i^0 (ref. 6).

Errors: Std. dev. $\sigma(T) = [\sum(T - T_{exp})^2/(N-n-2)]^{1/2}$,
Rel. std. dev. $100\sigma(\delta P/P) = 100[\sum((P - P_{exp})/P_{exp})^2/(N-n-2)]^{1/2}$,
 N , no. of exp. points, ref. 2,
 n , no. of coefficients in the smoothing equation.

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

EQUATIONS

$$G^E/RT = -x_1 \ln(x_1 + c_2 x_2) - x_2 \ln(x_2 + c_1 x_1)$$

$$c_1 = \exp \left[-(a_1 + \frac{a_2}{T}) \right] \quad c_2 = \exp \left[-(a_3 + \frac{a_4}{T}) \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1-y_i)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_i = P_i/P; \quad P_i^0/kPa = \exp [A_i + B_i / (C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2	
101.32	78.912 (28.4)	0 (0)	59.872 (28.1)	0 (0)	

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parentheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
101.32	15.33285	-3212.43	-90.41	12.44054	-2347.46	-116.55

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23, 147.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1978, k-5620, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsionopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.